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Microscopic dynamics of an amorphous C60x/C70(1 − x) fullerene mixture

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Abstract

© 2015, Pleiades Publishing, Ltd. This paper presents the results of investigation of the propagation mechanism of collective excitations in amorphous C60x/C70(1 − x) fullerene mixtures (with equimolar concentration x = 0.50), which were obtained using molecular dynamics simulation. The critical glass-transition temperature of the system Tc = 1548 K was determined from the change in the behavior of the Wendt-Abraham parameter. Spectral densities of the time correlation functions of the longitudinal (Formula presented.) and transverse (Formula presented.) currents for a wide region of wave numbers at temperatures below the glass-transition temperature were calculated. It was found that the dynamics of density fluctuations in amorphous C60x/C70(1 − x) fullerene mixtures is characterized by two dispersion acoustic-like branches of the longitudinal and transverse polarizations. The influence of poly-dispersity and form factor of the molecule of the mixture component on the microscopic dynamics of the density fluctuation in multicomponent systems was established.

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